Numerical Approximations of Phase Field Models using a General Class of Linear Time-Integration Schemes

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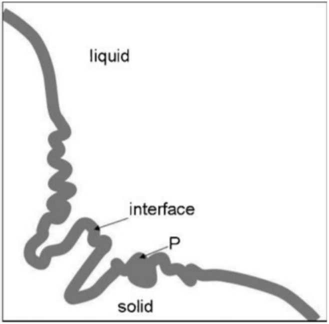
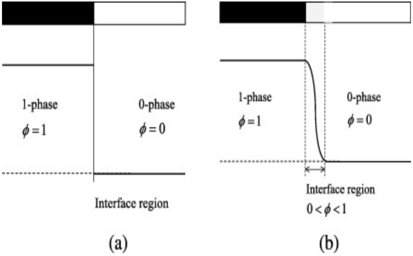
Outline

Background

Phase field model: A basic thermodynamical model that is used to describe phase separation process, microstructural evolution, etc. For example:





Phase Field Models

Total Energy:

$$E(t) = \int_\Omega \frac{\epsilon^2}{2}|\nabla\phi|^2 + f(\phi)d\mathbf{x}$$

where ϕ is a phase variable.

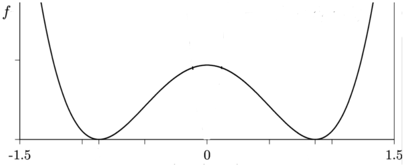


Figure: $f(\phi) = \frac{1}{4}(\phi^2 - 1)^2$

Energy Dissipation Law:

$$\frac{dE}{dt} = -(G\frac{\delta E}{\delta\phi}, \frac{\delta E}{\delta\phi}) \leq 0$$

General Phase Field Models:

$$\partial_t\phi(x,t) = -G\frac{\delta E}{\delta\phi} \quad \text{in } \Omega \times (0,T]$$

Phase Field Models

Allen-Cahn Model:

$$\phi_t = \epsilon^2 \Delta\phi - \phi^3 + \phi, \quad (\mathbf{x}, t) \in \Omega \times (0, T]$$

Nonlocal Allen-Cahn Model:

$$\phi_t = \epsilon^2 \Delta\phi - (\phi^3 - \phi) + \frac{1}{|\Omega|} \int_\Omega \phi^3 - \phi dx, \quad (\mathbf{x}, t) \in \Omega \times (0, T]$$

Cahn-Hilliard Model:

$$\phi_t = \Delta(-\epsilon^2 \Delta\phi + \phi^3 - \phi), \quad (\mathbf{x}, t) \in \Omega \times (0, T]$$

Energy Quadratization Method

EQ Method: Introduce an auxiliary variable to "remove" the nonlinear term from the energy density.

Allen-Cahn equation:

$$\phi_t = \epsilon^2 \Delta\phi - \phi^3 + \phi$$

Introduce

$$q := h(\phi) = \frac{1}{\sqrt{2}}(\phi^2 - 1 - \gamma)$$

Model Reformulation

$$\begin{cases} \phi_t = \epsilon^2 \Delta\phi - \gamma\phi - qg, \\ q_t = \dfrac{\partial q}{\partial \phi}\phi_t = g\phi_t \end{cases}$$

Numerical Schemes (Cont'd)

- Time Discretization (Crank-Nicolson Scheme)

$$\begin{cases} \dfrac{\phi^{n+1}-\phi^n}{\Delta t} = \epsilon^2 \Delta \phi^{n+\frac{1}{2}} - \gamma \phi^{n+\frac{1}{2}} - 2g(\phi^*) q^{n+\frac{1}{2}} \\ \dfrac{q^{n+1}-q^n}{\Delta t} = g(\phi^*) \dfrac{\phi^{n+1}-\phi^n}{\Delta t}, \quad \phi^* = \dfrac{3}{2}\phi^n - \dfrac{1}{2}\phi^{n-1} \end{cases}$$

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- Substitution

$$\phi^{n+\frac{1}{2}} = \frac{1}{2}(\phi^{n+1}+\phi^n), \quad q^{n+\frac{1}{2}} = \frac{1}{2}(q^{n+1}+q^n)$$

$$(\frac{2}{\Delta t} - \epsilon^2 \Delta + \gamma)\phi^{n+\frac{1}{2}} = \frac{2}{\Delta t}\phi^n - q^n g(\phi^*) - g^2(\phi^*)(\phi^{n+\frac{1}{2}} - \phi^n)$$

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- Space Discretization (Fourier Pseudospectral Method)

Numerical Experiment

Allen-Cahn Equation:

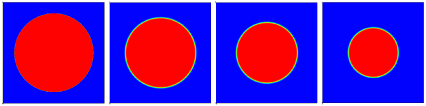

Figure: Time evolution of a disk driven by mean curvature at $t = 0$, 1000, 2000, 3000

Allen-Cahn Equation with the Volume Constraint:

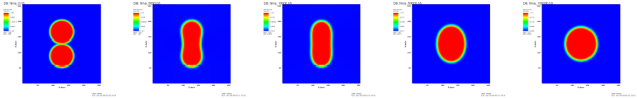

Figure: Time evolution of two kissing droplets emerging into a single one at $t = 0$, 0.005, 0.1, 0.5, 1

Thank you very much!